

Effect of series resistance and standard deviation on the nonlinear behavior of I-V characteristics in metal/conducting polymer Schottky diode

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Abstract : The current voltage characteristics of metal/conducting polymer Schottky diode are simulated using a Gaussian distribution of barrier height (BH), with a linear bias dependence. The calculated data are analyzed in order to get the effect of standard deviation (SD) on BH, activation energy and the ideality factor over the temperature range 100-300K. The analysis has been carried out using appropriate values of average of zero bias BH (ϕ_{b0}), and the two constant terms (γ and ξ) appearing from linear bias dependence of BH and SD. The chosen values of ϕ_{b0} , γ and ξ are selected from our earlier work on I-V measurements of metal/conducting polymer (Sn/PAN-PC) film. While the abnormal decrease of BH is due to SD, bias dependence of SD and BH account for the higher ideality factors at low temperatures. Also, the role played by diode series resistance for the non-linearity of the $\ln(I)$ -V plots is discussed.

Keywords : Conducting polymer, Schottky barrier, inhomogeneous barrier

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1. Introduction

The classical model of a metal semiconductor contact (Schottky diode) has a junction with a fixed barrier height (BH). However, such a description fails to account for the observed temperature dependence of current-voltage (I-V) characteristics on the basis of thermionic emission-diffusion (TED) theory. The discrepancies have, in fact, been attributed to the barrier inhomogeneities present in the Schottky diodes. For conventional inorganic semiconductors the barrier inhomogeneities are described with some distribution function, *e.g.* Gaussian or log normal [1-3]. The Gaussian distribution function is utilized to explain the difference in barrier heights observed from capacitance-voltage (C-V) and (I-V) measurements in several cases.

In our earlier work [4], assuming the Gaussian distribution of barrier height for metal/conducting polymer (Sn/PAN PC composite) junction, an attempt was made to explain the reason of abnormal decrease of BH and an increase of ideality factors (IF) at low temperatures. Average values of zero bias BH have been calculated for different temperatures in between 100-300K. As this parameter has been found to be almost temperature independent it justifies the significance of classical term 'fixed BH'.

An attempt is made here to simulate the I-V characteristics of metal/conducting polymer Schottky diodes on the basis of TED current equation [5], assuming a Gaussian distribution of barrier heights with linear bias dependence of its mean and standard deviation. The simulated I-V data are analyzed in details to examine the effects of distribution parameters and their bias dependences over a temperature range 100-300K. The aim is to identify the factors responsible for the abnormal decrease in BH and the simultaneous increase in IF with a decrease in temperature.

2. Method of analysis

According to TED theory, the basic equation for current density (J) of a Schottky diode is given by [4] :

$$J = A^* T^2 \exp(-q\phi_b / kT) [\exp\{q(V - IR_s) / kT\} - 1], \quad (1)$$

where ϕ_b is BH, R_s is series resistance and k and A^* are Boltzmann's and Richardson's constant.

Assuming the linear bias dependence of BH, *i.e.* $\phi_b = \phi_{b0} + \gamma V$, here ϕ_{b0} is zero bias BH and γ is the proportionality constant, eq. (1) modifies to :

$$J = J_0 \cdot \exp\{q(V - IR_s) / \eta kT\} [1 - \exp\{q(V - IR_s) / kT\}], \quad (2)$$

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where $J_0 = A^* T^2 \exp(-q\phi_{b0}/kT)$. (3)

J_0 is the saturation current at zero bias, and the modified ideality factor is given by

$$\eta = 1/(1-\gamma). \quad (4)$$

Now assuming Gaussian distribution of BH with a mean value $\bar{\phi}_b$ and standard deviation σ_s in the form

$$P(\phi_b) = 1/(\sigma_s(2\pi)^{1/2}) \exp[-(\bar{\phi}_b - \phi_b)^2 / 2\sigma_s^2]. \quad (5)$$

the total current density J in a forward bias V is given by

$$J(V) = \int_{-\infty}^{\infty} J(\phi_b, V) P(\phi_b) d\phi. \quad (6)$$

On integration,

$$J(V) = A^* T^2 \exp[-(q/kT)(\bar{\phi}_b - \sigma_s^2 q / 2kT)] \exp[q(V - IR_s)/kT] [1 - \exp(-q(V - IR_s)/kT)]. \quad (7)$$

Now, as we have incorporated in eq. (2) the bias voltage dependence, this should be extended to the entire Gaussian profile. Assuming linear bias dependence on Gaussian parameters $\bar{\phi}_b$ and σ_s , such as $\bar{\phi}_b = \bar{\phi}_{b0} + \gamma V$ and $\sigma_s = \sigma_0 + \xi V$ on substitution equation (7) becomes

$$J(V) = J_0 \exp[q(V - IR_s)/kT\eta_{ap}] \times [1 - \exp(-q(V - IR_s)/kT)], \quad (8)$$

where $J_0 = A_d A^* T^2 \exp(-q\phi_{ap}/kT)$. (9)

J_0 is the saturation current density, ϕ_{ap} and η_{ap} are apparent barrier height and ideality factor respectively and are given by the following equations:

$$\phi_{ap} = \bar{\phi}_{b0} - \sigma_0^2 q / 2kT, \quad (10)$$

$$1/\eta_{ap} = (1-\gamma) + \sigma_0 q \xi / kT. \quad (11)$$

Putting $\bar{\phi}_{b0} = 0.8$ eV, $\gamma = 0.80$ and $\xi = -0.010$ in eqs. (10) and (11), ϕ_{ap} and η_{ap} have been calculated with different σ_0 in the range of temperatures 100 to 300K. Now using eqs. (8) and (9), the values of current (I) have been calculated in the region of 0 to 4 volts. For different σ_0 , the plots of current (I) against voltage (V) are different and same thing also happened for different values of series resistance (R_s).

3. Results and discussion

The simulated $\ln(I) - V$ curves are shown in Figures 1 and 2 for various values of σ_0 and R_s at 200 and 300K. The plots of Figure 1 reveal that on increasing σ_0 , the linear region is gradually shortened. This behavior actually results due to the series resistance R_s associated with each elementary barrier. With an increase of σ_0 , more barriers of low barrier height (that

are effective) appear which, in turn, contribute increased current at any given bias.

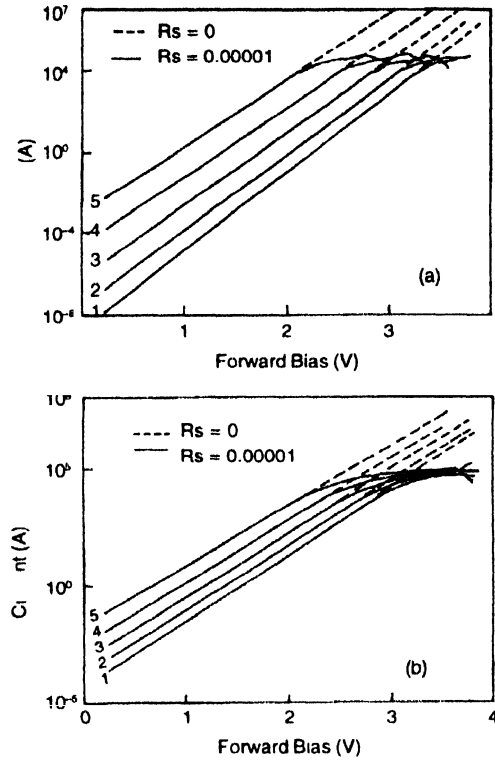


Figure 1. Simulated I-V characteristics for various values of standard deviation (σ_0) at temperatures (a) 200K and (b) 300K for different values of σ_0 (1 \rightarrow 0.08V, 2 \rightarrow 0.09V, 3 \rightarrow 0.1V, 4 \rightarrow 0.11V and 5 \rightarrow 0.12V).

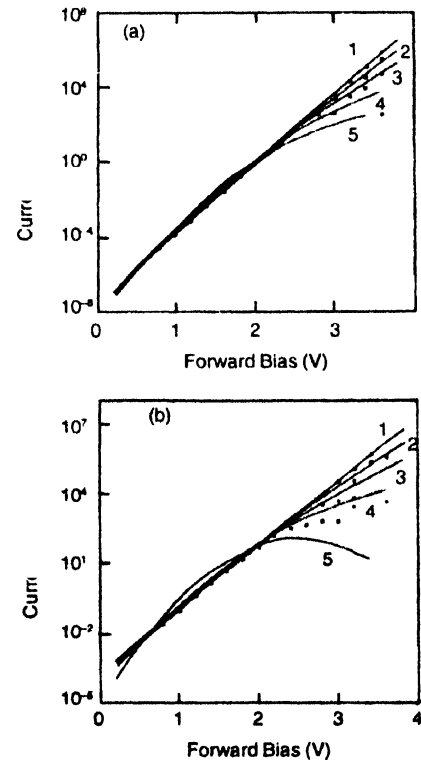


Figure 2. Simulated I-V characteristics for different values of series resistance (R_s) (1 \rightarrow 0.00, 2 \rightarrow 0.000001, 3 \rightarrow 0.00001, 4 \rightarrow 0.0001 and 5 \rightarrow 0.001) and standard deviation (σ_0) = 0.1 V at temperatures (a) 200K and (b) 300K.

The effect of R_s on $\ln(I) - V$ plots can easily be visualized from Figure 2 at two different temperatures viz 200 and 300K. Basically the reason for the nonlinearity in $\ln(I) - V$ plots are R_s . With increase in R_s the linearity breaks at lower values of forward bias whereas for zero value of R_s the plot is almost linear. The effect of R_s is not pronounced enough at low bias (upto 2.5 V for 200K and 2.0 V for 300K) when R_s is small. In real samples [4], R_s is much higher i.e., of the order of kilo-ohm at low temperature. In such cases, the deviation from straight line starts from a very low value of bias voltage.

The magnitudes of BH and IF are shown in Figures 3 and 4 respectively as a function of temperature for different σ_0 . Clearly as the temperature decreases, the BH decreases while the IF increases slowly at first but quite rapidly afterwards. Also, the

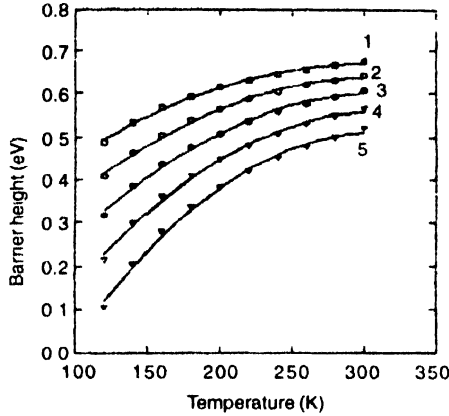


Figure 3. Variation of barrier height with temperature for different values of standard deviation (σ_0) (1 \rightarrow 0.08V, 2 \rightarrow 0.09V, 3 \rightarrow 0.1V, 4 \rightarrow 0.11V and 5 \rightarrow 0.12V)

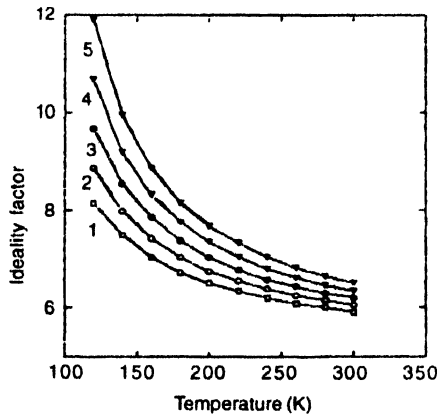


Figure 4. Variation of ideality factor with temperature at different values of standard deviation (σ_0) (1 \rightarrow 0.08V, 2 \rightarrow 0.09V, 3 \rightarrow 0.1V, 4 \rightarrow 0.11V and 5 \rightarrow 0.12V).

effects are greatly pronounced at larger values of σ_0 . The corresponding Richardson's plot (Figure 5) show similar characteristics. As the magnitude of σ_0 increases, the curve becomes more and more nonlinear. Indeed, from the experimental I-V data of metal/conducting polymer Schottky diode [4] the relevant curves match corresponding to $\sigma_0 = 0.10$.

Figures 6 and 7 show the variation of BH and IF as a function of σ_0 at different temperatures. In fact these curves follow eqs. (10) and (11). These parameters are less sensitive to the σ_0 at higher temperatures but become progressively more σ_0 dependent as the temperature is lowered. The relative change of BH is more for all the curves (i.e. temperatures) than IF. This is because as BH depends square of σ_0 (eq. (10)) where as IF

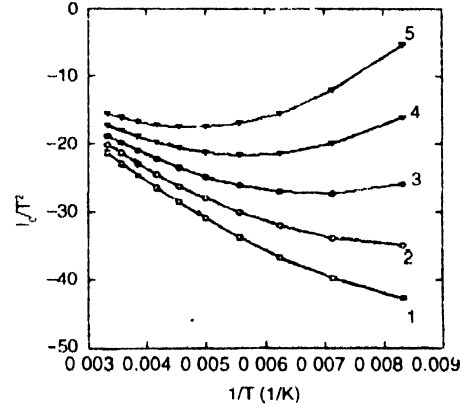


Figure 5. Plot of $\ln(J_0/T^2)$ with $1/T$ for different values of standard deviation (σ_0) (1 \rightarrow 0.08V, 2 \rightarrow 0.09V, 3 \rightarrow 0.1V, 4 \rightarrow 0.11V and 5 \rightarrow 0.12V)

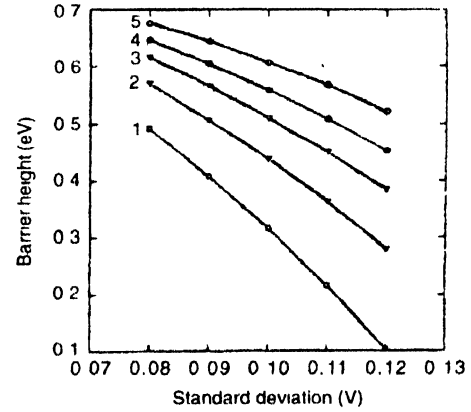


Figure 6. Variation of barrier height with standard deviation (σ_0) at different temperatures (1 \rightarrow 120K, 2 \rightarrow 160K, 3 \rightarrow 200K, 4 \rightarrow 240K and 5 \rightarrow 300K)

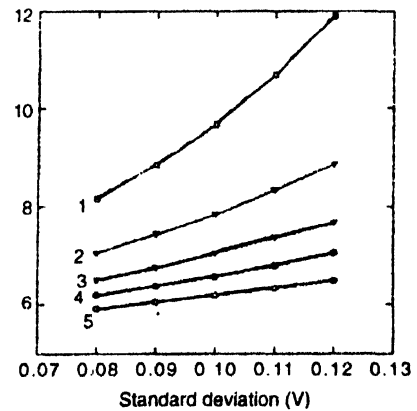


Figure 7. Variation of ideality factor with standard deviation (σ_0) at different temperatures (1 \rightarrow 120K, 2 \rightarrow 160K, 3 \rightarrow 200K, 4 \rightarrow 240K and 5 \rightarrow 300K).

varies linearly with σ_0 (eq. (11)). There is a multiplying factor ξ (eq. (11)) but the magnitude of ξ is less than σ_0 .

From the above discussion, it is clear that it is difficult to predict any universal relation between BH and IF. They depend on distribution function, which in turn, are function of chemistry, non-uniformity and other defect properties of the interface region. The effect is more pronounced at low temperature and that is why it is difficult to explain the low temperature data without assuming a distribution function of barrier height.

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